LA-UR -84-2947

CONF-850426--1

LA-UR--84-2947

DE85 002034

TITLE: A NUMERICAL MODEL FOR SIMULATING DYNAMIC PROCESSES IN ROCKS

MASTER

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SUBMITTED TO: 5th Int. Conf. on Numerical Methods in Geomechanics
April 1-5, 1985
Nagoya, Japan

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I. INTRODUCTION

We present a constitutive model for porous, brittle rocks that includes both compaction and fracture. The model is microphysical in that inelasticity is directly related to the mechanics of crack growth and also to the plastic collapse of spherical pores. The model is suitable for computing and has been implemented in a two-dimensional stress wave code.

In previous papers (Margolin 1983a; Margolin and Adams 1982), we have described the concept of the microphysical model and its essential components. These references are written in the context of a constitutive model for brittle materials, and so contain details of the generalized Griffith theory that governs the growth of penny-shaped cracks.

These subjects are again briefly discussed, but the present paper focuses primarily on new aspects of the model. In particular, we describe a mechanical model of pore collapse, the role of effective moduli in combining the effects of the pores and the cracks in a consistent fashion, and finally add some remarks on the importance of self-consistent corrections to the moduli in the calculation of spall.

II. MICROPHYSICAL MODELS

On a fine scale, a rock is not a continuum, but exhibits a variety of microstructure. Further, the inelastic response of solids can often be associated with changes in the microstructure. For example, brittle materials contain tiny embedded flaws. At certain levels of stress, these flaws can begin to grow, a process that we see macroscopically as fracture, and ultimately fragmentation. With this insight, one might hope that a constitutive model for brittle rocks would be based on fracture mechanics. However, most currently utilized constitutive models of inelastic behavior including fracture are macroscopic--i.e., are based on plasticity theory and ignore the microstructure.

Constitutive models that take account of microstructure are called microphysical models. These models contain two levels of description of the solid. On the large scale the models simulate an equivalent continuum. In most models, this continuum is elastic. However the effective moduli characterising the equivalent continuum vary with certain internal variables that are calculated from the microstructure of the small scale description.

On the small scale, the models contain a statistical description of the microstructure. Using mechanical models (for example, fracture mechanics if the structural elements are cracks), the microstructure evolves in time. Changes in the microstructure are driven by the macroscopic stress field.

Thus, these two levels of description are coupled interactively. The internal variables upon which the effective moduli depend are calculated from the state of the microstructure. The effective moduli are used to calculate the macroscopic stress field from the strain, which is determined external to the constitutive law. Finally, the macroscopic stress is used in the mechanical models to calculate changes in the microstructure in the small scale picture.

We emphasize that the microphysical approach does not require a detailed mapping of the actual microstructure in any problem. Rather, the microstructure is characterized statistically, and so represents a material property that can be determined in the laboratory. The microphysical model should be used for problems where the scales of interest are much larger than the intrinsic scales of the microstructure so that the medium really appears to respond as a continuum, and so that the statistics are "good".

The microphysical approach contains several advantages over other models based on plasticity theory. To begin, the input parameters of the microphysical model are physical properties that can be directly measured. Further, because the theory is based on physical parameters, it is capable of scaling in length and time. This is crucial because the strain-rate effect is extremely important in dynamic processes (see, for example, Grady and Kipp, 1979). Finally, the microphysical models are comparable to the plasticity models in terms of computational efficiency.

The particular model described in this paper is named PBCM (for porous-brittle constitutive model), and is intended for materials that exhibit both compaction and brittle failure. PBCM has been applied to rocks such as unsaturated tuffs and sandstones.

PBCM considers two types of microstructure--spherical pores and penny-shaped cracks. In Section III, we describe a mechanical model for the collapse of pores as a function of hydrostatic load. In Section IV, we review the generalised Griffith theory that determines when a crack may begin to grow as a function of crack size and orientation in a general stress field.

III. PORE COLLAPSE

Compaction is the inelastic (irreversible) loss of specific volume during the passage of a compressive stress wave. Microscopically, compaction is associated with the plastic collapse of pores. In this section, we describe a mechanical model for pore collapse, based mainly on the hollow sphere model of Carroll and Holt (1971).

Carroll and Holt consider spherical pores in an incompressible elastic-plastic material. They further assume that the system may be represented as a hollow sphere whose inner radius is the pore radius, and whose outer radius is chosen to match the material extension ratio α. Here, α is defined as the ratio of specific volume of the porous material to specific volume of the matrix material; α is a dimensionless number greater than or equal to one.

Carroll and Holt provide an analytic solution relating the time-dependent applied pressure on the outer boundary (with zero pressure on the inner boundary) to the resulting time-dependent extension ratio. The solution has three distinct branches in which the strain in the matrix material may be totally elastic, or partly elastic and partly plastic, or totally plastic. However, there is very little change of α in the first two phases.

The analysis contains two important parameters which are the yield stress, Y, of the matrix material, and a time scale that depends also on the yield stress as well as density, initial extension ratio, and initial pore radius. The result of the analysis is a second-order differential equation for α as a function of time.

PBCM was initially written to integrate this dynamic equation for α. However, in most cases of interest, the intrinsic time scale associated with pore collapse is much smaller than dynamic time scales associated with the stress wave. In such cases the inertial term in the pore collapse equation may be neglected, leaving the equilibrium relation

$$P \le \frac{2}{3} Y \ln \left(\frac{\alpha}{\alpha-1}\right) \qquad (1)$$

This equation governs the pore collapse. The "less-than-or-equal-to" sign means that α is a nonincreasing function of time.

In general, one might consider the effect of allowing a spectrum of pore sizes as would be found in the in situ rock. However, in the quasistatic case, the pore size does not appear in Eq. 1, and so it is sufficient to consider the average initial pore radius.

IV. FRACTURE

Much work has been done on the theory of fracture, most of which builds on the original ideas of Griffith (1920). The measured failure strength of brittle materials is often two orders of magnitude smaller than theoretical estimates based on breaking atomic bonds. Griffith postulated the existence of tiny flaws in brittle materials. The flaw tips act as stress concentrators, amplifying the external stresses to the point where the flaws begin to grow. Furthermore, a statistical distribution of flaw density as a function of size and orientation is a material property that can be determined directly by section and counting (Seaman, 1976).

Each microscopic flaw is really a tiny crack. It is crucial then to understand the conditions under which a crack may grow. Griffith's theory is based on the idea that the stability of the crack can be determined from general thermodynamic considerations. Griffith applied his analysis to two-dimensional slits in normal tension. The analysis has been generalized to three-dimensional penny-shaped cracks in spatially uniform, but otherwise arbitrary stress fields (Margolin, 1984).

For a crack in the x-y plane, the condition for growth is

$$\sigma_{zz}^2 + \left(\frac{2}{2-\nu}\right)\left(\sigma_{xz}^2 + \sigma_{yz}^2\right) > \frac{\pi T E}{2(1-\nu^2)c} \tag{2}$$

if σ_{zz} is tensile (positive) and

$$\left(\frac{2}{2-\nu}\right)\left(\sigma_{xz}^2 + \sigma_{yz}^2\right) > \frac{\pi T E}{2(1-\nu^2)c} \tag{3}$$

if σ_{zz} is compressive. Here c is the crack radius, ν is Poisson's ratio, E is Young's modulus, and T is the coefficient of surface tension. These equations show that smaller cracks are more stable, and that the effect of shear stress is to decrease the critical crack size for growth.

Unlike the situation with pores, it is always important to allow a spectrum of initial crack radii. This spectrum, coupled with the asymptotic limit on the speed of crack propagation, is the source of both size and strain-rate effects that characterize real geologic materials. The exact description of the evolution of a crack distribution with loading is a difficult problem, and many compromises must be made with the theory to render the model computable. PBCM uses a two-parameter analytic form to represent the crack distribution as it evolves. Details can be found in Demuth, et al. (1984).

V. EFFECTIVE MODULI

The presence of cracks and pores alters the elastic response of the material. The effective moduli represent the elastic properties of an equivalent continuous medium. Effective elastic moduli are substantially different from the tangent moduli. Tangent moduli are calculated from the slope of a stress-strain curve during inelastic deformation, and so depend critically on the history of loading. By contrast, the effective elastic moduli depend only on the instantaneous state of the microstructure.

The effective elastic moduli are found from static solutions of the displacement field for a body with a (statistically) prescribed microstructure, and subject to a macroscopically uniform stress field. To lowest order, the total strain of the body is the sum of the elastic strain of the matrix material plus the extra strain due to opening and shearing of the cracks and pores. The elastic strain of the matrix is simply related to the stress if the matrix is assumed to be linear elastic. The response of a single crack or pore to uniform stress is found from detailed solutions in Sneddon (1969) and Mackenzie (1950).

To derive the total effect of the microstructure, one must then sum up the effects of the individual cracks and pores over the entire microstructure. This summing process leads to several dimensionless numbers which we term internal variables. These internal variables form the connection between the microscopic and macroscopic levels of the constitutive model.

One of these internal variables is the extension ratio, α. The other variable, γ, represents the third moment of the crack density distribution. For example for a simple material containing only cracks bedded parallel to the x-y plane, the effective compliance C_{zzzz} is related to the compliance of the matrix material C^{o}_{zzzz} by (Margolin, 1983b).

$$C_{zzzz} = C^{o}_{zzzz} \left(1 + \frac{16}{3} (1 - \nu^2)\gamma\right) \quad . \tag{4}$$

This equation shows that the cracked material is softer than the uncracked material. For more general crack distributions, γ becomes a two-index tensor.

The essence of the effective moduli is that they enable us to write stress as a function of strain plus the internal variables. The constitutive law is exactly integrable in time--i.e., is an equation of state--and depends on the history only through the internal variables.

Furthermore, all inelasticity in our model results from the evolution of the microstructure. In rate form, the constitutive law has the form

$$\frac{d\varepsilon_{ij}}{dt} = \frac{d}{dt} \left(C_{ijkl}\sigma_{kl}\right) \tag{5}$$

Inverting for the stress rate

$$\frac{d\sigma_{kl}}{dt} = \left(C^{-1}\right)_{klij} \left[\frac{d\varepsilon_{ij}}{dt} - \sigma_{mn} \frac{dC_{ijmn}}{dt}\right] \tag{6}$$

Thus, the constitutive relation has the form of a viscoelastic solid, and the relaxation time is determined by the rate of change of the internal variables.

The effective moduli described above are derived for bodies whose pores and cracks are relatively far apart. To be precise, in the derivation of the effective moduli, we have assumed

$$\gamma \ll 1 \qquad ; \qquad (\alpha - 1) \ll 1 \tag{7}$$

For larger values of these internal variables, self-consistent field corrections must be applied to the moduli (Hoenig, 1979).

The effect of the self-consistent corrections is to predict softer elastic response for large values of $(\alpha - 1)$ and much more rapid softening of the material during crack growth. The latter is important in calculations involving rapid fracture to correctly describe localization effects. A particular example is the spall calculation of the last section.

V. IMPLEMENTATION

PBCM has been implemented in the computer program SHALE (Demuth, et al. 1984). SHALE is a finite difference code that integrates the equations representing conservation of mass, momentum, and energy in a continuum. The conservation laws must be supplemented by a constitutive law, a thermodynamic relation between the deformation of the medium and the restoring forces (that is, the stress field). The conservation equations and the constitutive equation form a complete set which, with appropriate boundary and initial conditions, describe the behavior of the continuum.

SHALE is based on a time marching procedure. Given the values of all the field variables at any time, SHALE approximately integrates the equations over a small increment of time to find the field variables at the later time. The increment of time is called the time step, and integration of the equations over a time step is termed a computational cycle.

In the first step of the computational cycle, strain rates are calculated from the spatial gradients of material velocity. Next, PBCM is called to update the stress tensor. With the time-advanced stresses, accelerations and the new material velocity field can be calculated. Finally, with the new velocities, time-advanced positions, densities, and internal energies can be computed.

Within PBCM, the internal variables associated with compaction and fracture must be updated. A brittle material contains cracks with a variety of sizes and orientations. PBCM assumes that the competent rock contains a distribution of cracks as a function of size. Angular variations are represented by discrete bins. Initially, the distribution is a material property. As the material is loaded, the distribution evolves using the generalized Griffith criteria [Eq. (2) and (3)] to determine which cracks may grow. The actual distribution becomes quite complicated; however, PBCM approximates the true distribution with a simple two-parameter fit. Details may be found in Demuth, et al. (1984).

One must be careful in treating the cracks to recognize that the effective moduli are discontinuous between normal tension and compression. This reflects the physical situation that, in normal tension, cracks open proportionately to the stress. However, in normal compression, cracks can do no more than close.

Under most circumstances, crack growth is an unstable process. That is, stress relaxation associated with growth is more than offset by the lower stress levels required to propagate bigger cracks. This means we can calculate crack growth explicitly--independent of the final stress state.

The situation is more complicated during pore closure. As a nearly equilibrium process, the final pressure and extension ratio must be related by Eq. (1) during compaction. The first step in updating α is to calculate the new pressure elastically, allowing no compaction. Then one checks whether this elastic estimate exceeds the critical pressure given in Eq. (1) based on the current value of α. If it does not exceed the critical value, no compaction occurs and the elastic calculation applies. Otherwise, one must simultaneously solve Eq. (1) along with the equation

$$p = -K_e \varepsilon_{ii} \tag{8}$$

Here, K_e is the effective bulk modulus which depends on α.

Equation (1) represents the allowable pairs (p,α) based on the Carroll-Holt model of pore collapse. Equation (7) describes the partition of strain between matrix material and pores. Regarding the dilatation ε_{ii} as known, these two equations can be solved simultaneously for the updated pressure p and the extension ratio α.

One more important detail concerns the measure of strain. Most stress wave codes identify the strain with the symmetrized velocity gradients

$$\frac{d\varepsilon_{ij}}{dt} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) \tag{9}$$

However, the effective moduli are defined as elastic moduli of the material at a given state of the microstructure. If the microstructure changes during a computational cycle, the appropriate strain rate must properly reflect changes in the reference (unloaded) state of the material. This is particularly important during compaction when most of the apparent volume change is associated with compaction, and hence, with permanent change in reference state. Instead of Eq. (8), the appropriate strain rate for PBCM is

$$\frac{d\varepsilon_{ij}}{dt} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) - \frac{1}{\alpha_o}\frac{d\alpha_o}{dt}\varepsilon_{ij} \qquad (10)$$

where α_o is the extension ratio of the reference state.

SHALE with PBCM has been applied to the problem of calculating ground motion from a deeply buried nuclear explosion. The problem starts with detonation of a nuclear explosive, sending strong stress waves through the ground. The aim of the calculation is to predict time histories of velocity and acceleration at the surface.

The phenomena that SHALE must represent are complex. Close to the detonation point, energy mainly in the form of radiation couples into the ground producing a region of melted and vaporized rock. These processes generate a strong compressive stress wave which propagates away from the detonation point. Outside the melted region, the wave propagates inelastically for a while and, after sufficient attenuation, elastically. The inelasticity is associated with compaction. Inelasticity and spherical divergence cause the wave to disperse and attenuate.

The compressive wave reflects from the surface as a tensile wave. Rapid, localized fracture accompanies the first appearance of tension, approximately one-half wavelength of the pulse below the ground. The fractures in this region coalesce, and completely separate the spall layer from underlying rock. The spall layer is thrown up and then falls only under the influence of gravity. Finally, it hits the underlying rock and bounces.

The figure shows the surface vertical velocity history of a particularly simple test problem chosen to isolate these physical processes. A quasi-one-dimensional stack of cells was initialized with overburden stress, and a Gaussian stress pulse with a width of 10 msec was imposed at the bottom boundary (300 m) at zero time. This pulse shape is a realistic approximation to the loading from an underground explosion. The pulse reflects from the surface, causing an upward acceleration, and the reflected tensile pulse causes spall at depth. The strong rebound from peak velocity lasts while cracks grow and cause the formation of a new free surface at the spall gap. The velocity curve turns into a straight slope as the spall layer decreases velocity during its free fall period under the influence of gravity, then returns to zero velocity in a series of bounces.

In summary, we have implemented a fracture and failure model based on the correct microphysical basis for fracture, and reproduced the correct set of spall, free fall, and slapdown phenomena without numerical art'fices or ad hoc modifications to our code. Furthermore, the correct scaling and strain rate dependences are built into our model.

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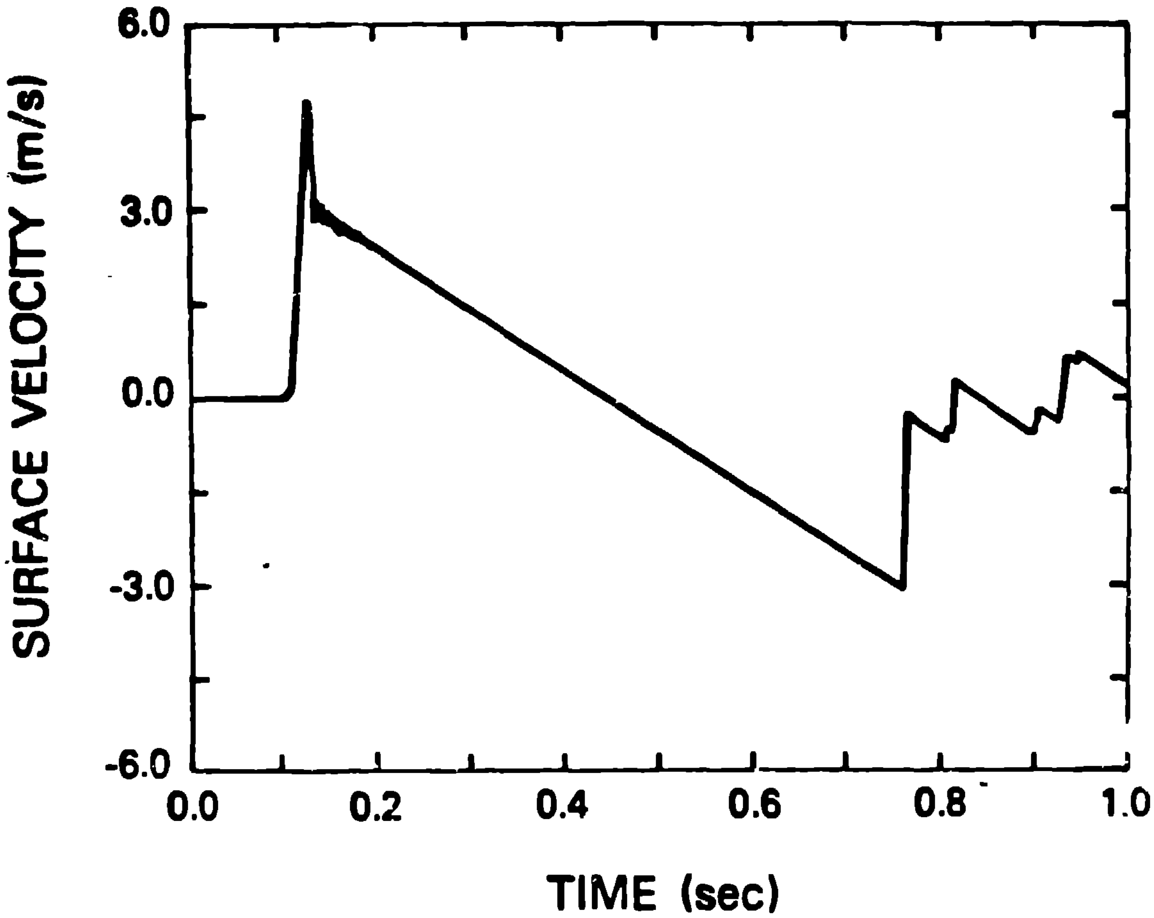

Figure: Surface velocity history in SHALE/BCM test calculation.